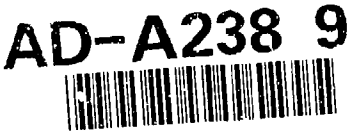

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AN EXPLOSIVES PRODUCTS THERMODYNAMIC EQUATION OF STATE APPROPRIATE FOR MATERIAL ACCELERATION AND OVERDRIVEN DETONATION: THEORETICAL BACKGROUND AND FORMULATION

Ernest L. Baker

July 1991

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Many modern explosive applications require modeling of both overdriven detonation and lower pressure detonations products expansion. Common thermodynamic equations of state used for warheads design have been demonstrated to provide poor representations of overdriven detonation. The Jones-Wilkens-Lee-Baker (JWLB) has been formulated to provide a more accurate representation. This report provides a detailed theoretical background and equation of state formulation for JWLB.

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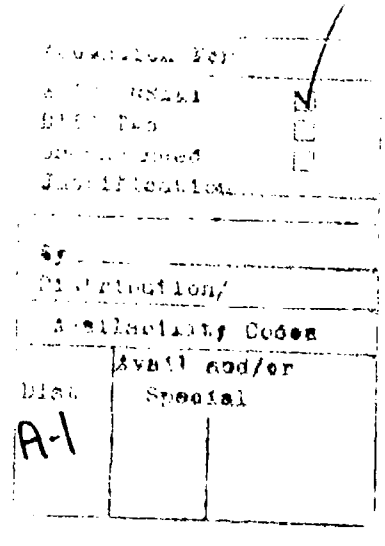

BACKGROUND

Many modern explosive applications require finite element and finite difference modeling of both overdriven detonation and lower pressure detonation products expansion. Large detonation wave shaping and multiple point initiation are typical overdriven detonation applications. Lower pressure detonation products expansion is required for material acceleration applications, such as explosively formed penetrators and shaped charges. Current thermodynamic equation of states used in dynamic finite element and finite difference programs are either parameterized to give agreement with thermochemical calculations [1] or experimental copper cylinder explosive expansion experiments [2,3]. Thermochemical calculations have proven to be very useful for the prediction of explosive products properties, particularly near and above the Chapman-Jouguet state [4,5]. Unfortunately, they do not reproduce the products expansion behavior accurately enough for typical warheads design. Currently, thermodynamic equations of state (JWL, Wilkens) [2,3] used for warheads design are normally calibrated to give agreement with copper cylinder explosive expansion experiments. These equations of state have not been calibrated for high pressures above the Chapman-Jouguet state. Experimentation [6] and comparison with thermochemical calculations (Figures 1,2, and 3) have demonstrated that a poor description of the high pressure region exists. In order to achieve a suitable equation of state for both overdriven and lower pressure products expansion, an appropriate equation of state form has been derived. A previous preliminary report [7] briefly describes the equation of state and parameterization methodology, but does not include details. This report provides a detailed theoretical background and equation of state formulation. A forthcoming report will provide a detailed description of the parameterization methodology.

EQUATION OF STATE FORMULATION

The equation of state form was chosen so as to adequately describe the high pressure regime produced by overdriven detonation, and yet retain the low pressure expansion behavior required for standard material acceleration modeling. To this end, the derived form is based on the Jones-Wilkens-Lee (JWL) equation of state [1] due to its computational robustness, and asymptotic approach to an ideal gas at high expansions. Additional exponential terms and a variable Gruneisen parameter have been added to adequately describe the high pressure region above the Chapman-Jouguet state. The resulting equation of state form, named Jones-Wilkens-Lee-Baker (JWLB), is

$$P = \sum_i A_i \left[1 - \frac{\lambda}{R_i V}\right] e^{-R_i V} + \frac{\lambda E}{V} + C\left(1 - \frac{\lambda}{\omega}\right) V^{-(\omega+1)} \qquad (1)$$

where,

$$\lambda = \sum_i (A_{\lambda i} V + B_{\lambda i}) e^{-R_{\lambda i} V} + \omega \qquad (2)$$

For consistency with the JWL equation of state, V is defined as a specific volume ratio, $V \equiv$

ρ_o/ρ and E is defined as $E = \rho_o e$ where e is the specific internal energy. The JWLB equation of state form is based on a first order expansion around the principal isentrope:

$$P_s = \sum_i A_i e^{-R_i V} + C V^{-(\omega+1)}. \tag{3}$$

Using the Gruneisen Parameter,

$$\lambda = V \left.\frac{\partial P}{\partial E}\right|_V, \tag{4}$$

the isentropic identity,

$$P = - \left.\frac{\partial E}{\partial V}\right|_s \tag{5}$$

$$\Rightarrow E_s - E_{cj} = \sum_i \frac{A_i}{R_i} e^{-R_i V} + \frac{C}{\omega} V^{-\omega} - \sum_i \frac{A_i}{R_i} e^{-R_i V_{cj}} - \frac{C}{\omega} V_{cj}^{-\omega}, \tag{6}$$

and the Chapman-Jouguet condition,

$$E_{cj} = E_o + \frac{1}{2}(P_{cj} + P_o)(V_o - V_{cj})$$

$$= \sum_i \frac{A_i}{R_i} e^{-R_i V_{cj}} + \frac{C}{\omega} V_{cj}^{-\omega}, \tag{7}$$

the final form may be derived

$$P = \frac{\lambda}{V}(E - E_s) + P_s$$

$$= \frac{\lambda}{V}\left(E - \sum_i \frac{A_i}{R_i} e^{-R_i V} - \frac{C}{\omega} V^{-\omega}\right) + \sum_i A_i e^{-R_i V} + C V^{-(\omega+1)} \tag{8}$$

$\Rightarrow$ Final Form.

Some important characteristics of the equation of state are that the Gruneisen Parameter λ, is represented as an analytic function of specific volume, V. $\lambda + 1$ approaches a constant adiabatic gamma, $\left.\frac{V}{P}\frac{\partial P}{\partial V}\right|_s = \omega + 1$ for large V, so that ideal gas behavior is asymptotically approached. The principal isentrope description is essentially identical to JWL, with the exception of an increased number of exponential terms. It has been found that for most explosives, three exponential terms (instead of two in JWL) are adequate to describe the principal isentrope over both the high pressure region above the Chapman-Jouguet state and the lower pressure expansion region. It is important to note that the internal energy referencing is defined by (7). The value of E_o must be consistent so that,

$$E_o = \sum_i \frac{A_i}{R_i} e^{-R_i V_{cj}} + \frac{C}{\omega} V_{cj}^{-\omega} - \frac{1}{2}(P_{cj} + P_o)(V_o - V_{cj}) . \qquad (9)$$

Normally, the equation of state parameters are chosen so that E_o has the value $E_o = \rho_o \Delta H$, where ΔH is the heat of detonation. This is consistent with the initial internal energy of the unreacted material having a value of zero.

SPEED OF SOUND

The generalized speed of sound is often required for implementation into a finite element or finite difference program. The speed of sound may be easily derived as follows,

$$\frac{\partial P}{\partial V} = \sum_i A_i \left[\frac{\lambda}{R_i V^2} - \frac{\frac{\partial \lambda}{\partial V}}{R_i V} \right] e^{-R_i V} - \sum_i A_i \left[1 - \frac{\lambda}{R_i V} \right] R_i e^{-R_i V}$$

$$+ C \left(- \frac{\frac{\partial \lambda}{\partial V}}{\omega} \right) V^{-(\omega+1)} - C(\omega + 1)\left(1 - \frac{\lambda}{\omega}\right) V^{-(\omega+2)}$$

$$- \frac{E\lambda}{V^2} + \frac{\lambda}{V} \frac{\partial E}{\partial V} + \frac{E}{V} \frac{\partial \lambda}{\partial V} \qquad (10)$$

$$(5), (10) \Rightarrow \left. \frac{\partial P}{\partial V} \right|_S = \sum_i A_i \left[\frac{\lambda}{R_i V^2} - \frac{\frac{\partial \lambda}{\partial V}}{R_i V} - R_i + \frac{\lambda}{V} \right] e^{-R_i V}$$

$$- C \left[(\omega+1)\left(1 - \frac{\lambda}{\omega}\right) + V \frac{\frac{\partial \lambda}{\partial V}}{\omega} \right] V^{-(\omega+2)}$$

$$- \frac{E\lambda}{V^2} - \frac{\lambda}{V} P + \frac{E}{V} \frac{\partial \lambda}{\partial V} \qquad (11)$$

$$c^2 = \frac{\partial P}{\partial \rho} \Rightarrow \rho_o c^2 = -V^2 \left. \frac{\partial P}{\partial V} \right|_S \qquad (12)$$

$$\Rightarrow \rho_o c^2 = \sum_i A_i \left[V \frac{\frac{\partial \lambda}{\partial V}}{R_i} - \frac{\lambda}{R_i} + R_i V^2 - \lambda V \right] e^{-R_i V}$$

$$+ C \left[(\omega+1)\left(1 - \frac{\lambda}{\omega}\right) + V \frac{\frac{\partial \lambda}{\partial V}}{\omega} \right] V^{-\omega} + E\lambda + \lambda V P - E V \frac{\partial \lambda}{\partial V} \qquad (13)$$

$$\frac{\partial \lambda}{\partial V} = \sum_i A_{\lambda i} e^{-R_{\lambda i} V} - \sum_i (A_{\lambda i} V + B_{\lambda i}) R_{\lambda i} e^{-R_{\lambda i} V} \qquad (14)$$

ADIABATIC GAMMA

Another useful quantity is the generalized adiabatic gamma. The adiabatic gamma may also be easily derived,

$$\gamma \equiv -\left.\frac{\partial \ln P}{\partial \ln V}\right|_s = -\left.\frac{V}{P}\frac{\partial P}{\partial V}\right|_s \tag{15}$$

$$(11), (15) \Rightarrow \gamma = \frac{1}{P}\sum_i A_i\left[\frac{\frac{\partial \lambda}{\partial V}}{R_i} - \frac{\lambda}{R_i V}\frac{\frac{\partial \lambda}{\partial V}}{R_i} + R_i V - \lambda\right]e^{-R_i V}$$

$$+ \frac{C}{P}\left[(\omega+1)\left(1-\frac{\lambda}{\omega}\right) + V\frac{\frac{\partial \lambda}{\partial V}}{\omega}\right]V^{(\omega+1)} + \frac{E\lambda}{VP} + \lambda - \frac{E}{P}\frac{\partial \lambda}{\partial V} \tag{16}$$

$$(14) \Rightarrow \frac{\partial \lambda}{\partial V} = \sum_i A_{\lambda i} e^{-R_{\lambda i} V} - \sum_i (A_{\lambda i} V + B_{\lambda i}) R_{\lambda i} e^{-R_{\lambda i} V}.$$

PRINCIPAL ISENTROPE PROPERTIES

Often, properties along the isentrope that passes through the Chapman-Jouguet state are of particular interest. The Gruneisen parameter is given by (2). The adiabatic gamma is given by,

$$(3) \Rightarrow \frac{\partial P_s}{\partial V} = -\sum_i A_i R_i e^{-R_i V} - C(\omega+1)V^{(\omega+2)} \tag{17}$$

$$(3), (15) \Rightarrow \gamma_s = \frac{V\sum_i A_i R_i e^{-R_i V} + C(\omega+1)V^{(\omega+1)}}{\sum_i A_i e^{-R_i V} + CV^{(\omega+1)}}. \tag{18}$$

The speed of sound along the principal isentrope is given by,

$$(12) \Rightarrow \rho_0 c^2 = \sum_i A_i R_i V^2 e^{-R_i V} + C(\omega+1)V^{\omega}. \tag{19}$$

REACTED PRODUCTS HUGONIOT

Another often used state space locus is the reacted products Hugoniot. Assuming the initial pressure to be zero, conservation gives,

Mass: $\rho_0 D = \rho(D-u)$ (20)

Momentum: $P = \rho_0 D u$ (21)

Energy: $$\frac{D^2}{2} + \frac{E_0}{\rho_0} = \frac{P}{\rho} + \frac{(D-u)^2}{2} + \frac{E}{\rho_0} \tag{22}$$

$$(20) \Rightarrow u = \frac{\rho - \rho_o}{\rho} D = (1-V)D \tag{23}$$

$$(23),(20) \Rightarrow P = \rho_o(1-V)D^2 \Rightarrow D^2 = \frac{P}{\rho_o(1-V)} \tag{24}$$

$$(22),\ (24) \Rightarrow \frac{P}{2\rho_o(1-V)} + \frac{E_o}{\rho_o} = \frac{P}{\rho} + V^2\frac{P}{2\rho_o(1-V)} + \frac{E}{\rho_o} \tag{25}$$

$$\Rightarrow E = E_o + \frac{P}{2(1-V)} - V^2\frac{P}{2(1-V)} - PV$$

$$= E_o + \frac{P}{2(1-V)}(1-V^2-2V+2V^2) = E_o + \frac{P}{2(1-V)}(V^2-2V+1)$$

$$= E_o + \frac{P(1-V)}{2} \tag{26}$$

$$(1),\ (26) \Rightarrow E\left(1 - \frac{\lambda(1-V)}{2V}\right)$$

$$= E_o + \left(\sum_i A_i\left[1 - \frac{\lambda}{R_i V}\right]e^{-R_i V} + C\left(1 - \frac{\lambda}{\omega}\right)V^{(\omega+1)}\right)\frac{(1-V)}{2} \tag{27}$$

$$\Rightarrow E = \frac{E_o + \left(\sum_i A_i\left[1 - \frac{\lambda}{R_i V}\right]e^{-R_i V} + C\left(1 - \frac{\lambda}{\omega}\right)V^{(\omega+1)}\right)\frac{(1-V)}{2}}{\left(1 - \frac{\lambda(1-V)}{2V}\right)} \tag{28}$$

CONCLUSION

An advanced thermodynamic equation of state applicable to problems involving overdriven detonation and material acceleration has been developed and calibrated for several explosives. This manuscript has presented a theoretical background and formulation for the new equation of state. A forthcoming report will describe the parameterization methodology. The new equation of state maintains required low pressure expansion behavior while providing a better high pressure description applicable to overdriven detonation. Typical applications of the new equation of state include wave shaped and peripherally initiated munitions. Finally, the equation of state asymptotically approaches the constant gamma equation of state at high expansions. It is therefore believed that the equation of state will be applicable to extremely large volume expansion applications, such as blast, without a loss of accuracy in the higher pressure regions. In order to use the equation of state for very large expansions, proper calibration to very large volume expansion experimentation will be required.

SYMBOLS

$P \equiv$ Pressure

$\rho \equiv$ Density

$V \equiv$ Ratio of Specific Volume to Initial Specific

V ≡ Volume

E ≡ Specific Internal Energy divided by Initial Specific Volume

λ ≡ Gruneisen Parameter

γ ≡ Adiabatic Gamma

c ≡ Sound Speed

D ≡ Detonation Velocity

u ≡ Mass Velocity

ΔH ≡ Heat of Detonation

A_i, R_i, C, $A_{\lambda i}$, $B_{\lambda i}$, $R_{\lambda i}$, ω ≡ Equation of State Constants

$_s$ ≡ Isentropic

$_{cj}$ ≡ Chapman-Jouguet State

$_o$ ≡ Initial Conditions

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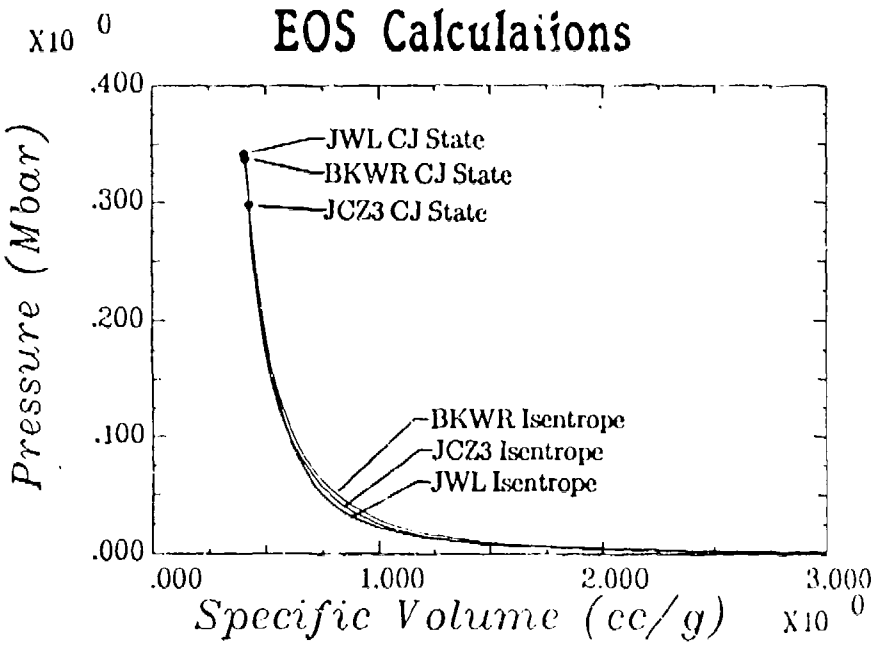

Figure 1. Pressure versus specific volume for the principal isentrope of octol 75/25 below the Chapman-Jouguet state. The thermochemical calculations (BKWR and JCZ3) agree fairly well with the standard JWL.

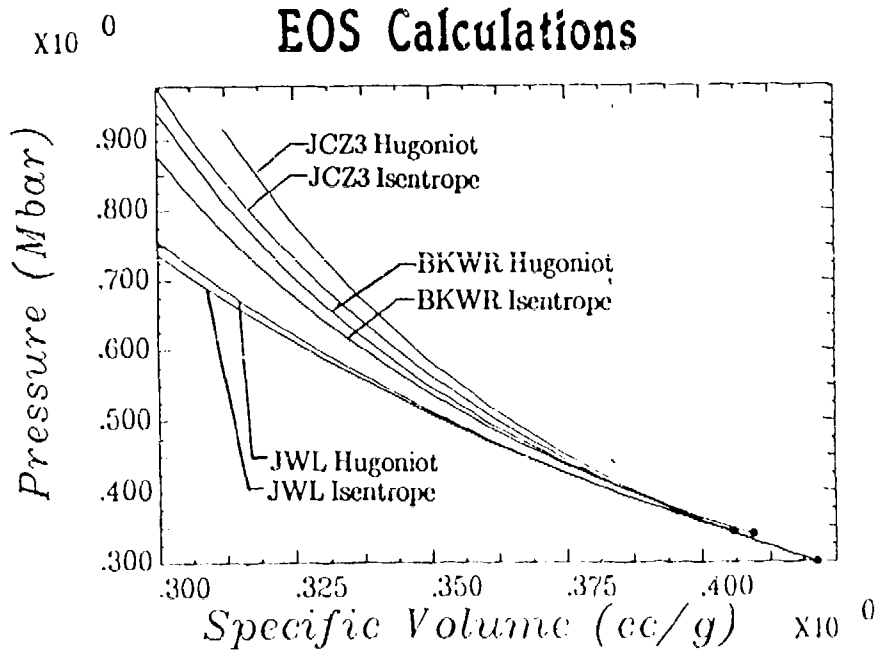

Figure 2. Pressure versus specific volume for the principal isentrope and reactive Hugoniot of octol 75/25 above the Chapman-Jouguet state. The standard JWL underpredicts the high pressure region.

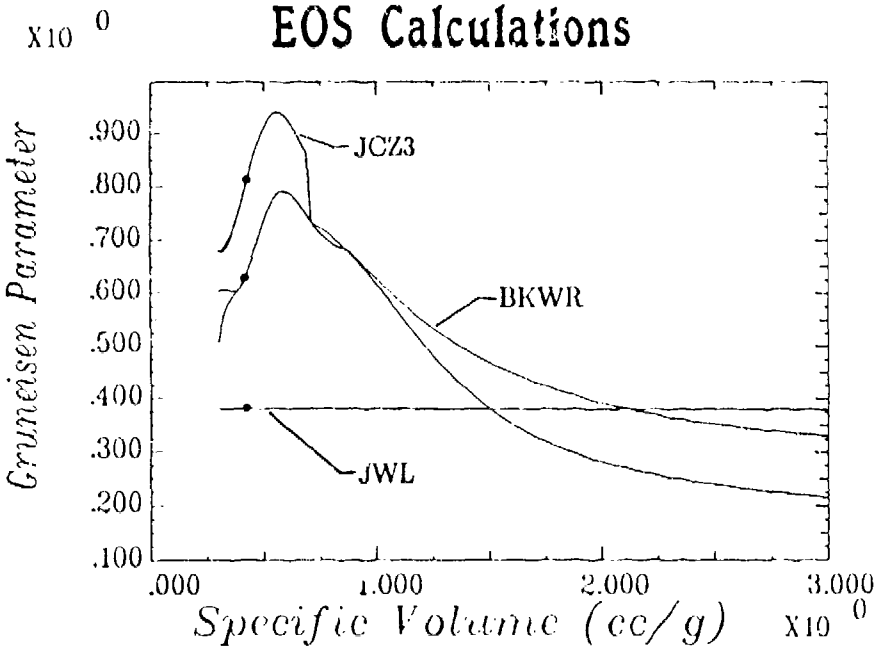

Figure 3. The Gruneisen parameter versus specific volume for the principal isentrope and reactive Hugoniot.

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